

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property
Organization
International Bureau



(43) International Publication Date
18 March 2004 (18.03.2004)

PCT

(10) International Publication Number
WO 2004/023349 A2

(51) International Patent Classification⁷: **G06F 17/50**

Discovery Limited, Spierlla Buildings, Suite 203, Bridge Road, Letchworth, Hertfordshire SG6 4ET (GB).

(21) International Application Number:
PCT/GB2003/003605

(74) Agent: **D YOUNG & CO**; 21 New Fetter Lane, London EC4A 1DA (GB).

(22) International Filing Date: 18 August 2003 (18.08.2003)

(81) Designated States (*national*): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
0220785.0 6 September 2002 (06.09.2002) GB

(71) Applicant (*for all designated States except US*): **CRESSET BIOMOLECULAR DISCOVERY LIMITED** [GB/GB]; Spierlla Buildings, Suite 203, Bridge Road, Letchworth, Hertfordshire SG6 4ET (GB).

(84) Designated States (*regional*): ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

(72) Inventors; and

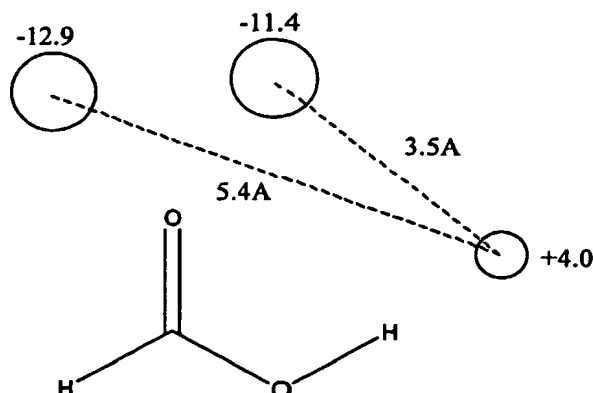
(75) Inventors/Applicants (*for US only*): **CHEESERIGHT, Tim** [GB/GB]; c/o Cresset Biomolecular Discovery Limited, Spierlla Buildings, Suite 203, Bridge Road, Letchworth, Hertfordshire SG6 4ET (GB). **MACKEY, Mark, Denis** [AU/GB]; c/o Cresset Biomolecular Discovery Limited, Spierlla Buildings, Suite 203, Bridge Road, Letchworth, Hertfordshire SG6 4ET (GB). **VINTER, Jeremy, Gilbert** [GB/GB]; C/O Cresset Biomolecular

Published:

— *without international search report and to be republished upon receipt of that report*

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: COMPARISON OF MOLECULES USING FIELD POINTS



(57) **Abstract:** A method of comparing two conformers in which an overlay score is obtained by determining the field value for molecule A at the coordinates of molecule B's field point. Molecule B's field point does not have to be very close to molecule A's field point to get a good overlay score: it just needs to be in a region where molecule A's field is large. This overcomes a limitation of conventional pseudo-Coulombic scoring in which a low score is achieved when extrema of large extent overlap but have their minimum points widely separated. The method can be applied to molecular mechanics modelling using atom centred charges (ACCs) and extended electron distributions (XEDs) as well as to quantum mechanics models.